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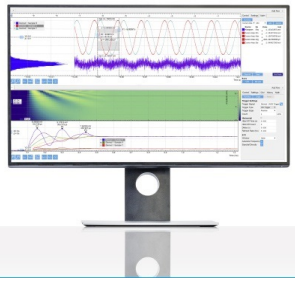

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ABSTRACT

Oxygen and hydrogen are the two most important impurities in semiconductors because of their ubiquitous presence in growth and device processing environments, and consequently, their incorporation strongly influences electronic and electrical properties. Therefore, a deeper understanding of the interaction of these species with the semiconductor surface and bulk defects is necessary for enabling the development of devices based on them, such as photovoltaic and photocatalytic systems and fuel cells. It is shown here, through the analysis of the reported surface work function values and substitutional bulk O-defect energies, that the surface Fermi level of semiconductors with physisorbed O_2 lies universally at approximately −5.1 eV below the vacuum level. Similarly, the results show that the energy of substitutional bulk O-related amphoteric defects incorporated during the crystal growth also has a universal energy of ∼−5.0 eV with respect to the vacuum level for most semiconductors investigated. It is shown that the process of "surface transfer doping" involving an adsorbed water film on the semiconductor surface is likely responsible for the universal alignment of oxygen levels.

Lattices of most semiconductors have a large density of intrinsic and extrinsic defects, which gives rise to effects such as surface Fermi level (E_F) pinning, dopant compensation, asymmetrical p vs n-doping, and device degradation. Phenomenological models[1–4] have been proposed for systematization and prediction of doping and E_F pinning behavior in semiconductors. These include (i) "doping limit rule" that assigns the lower (p-type, E^p_{pin}) and upper (n-type, E^n_{pin}) bounds for the E_F pinning position to defects such as cation vacancies and Si-DX centers.[1] Remarkably, the E^p_{pin} and E^n_{pin} energies in various III–V and II–VI compounds are universally constant when compared with respect to the energy of the vacuum level (E_{VAC}); (ii) "amphoteric defect model" that assigns the E_F pinning to amphoteric intrinsic defect pairs, such as the $V^{2-}_{Ga}/(As_{Ga} + V_{As})^{3+}$ defect complex in GaAs, formed through lattice atom migration and is capable of transforming from acceptor-type to donor-type and vice versa.[3] Similar to the E_{pin} values, the calculated E_F pinning position, which is taken as the Fermi stabilization energy (E_{FS}), is reported to be a constant with a universal energy of 4.9 eV below E_{VAC}; and (iii) amphoteric negative-U interstitial hydrogen defect (H^+/H^-) with a constant universal value of ∼−4.5 eV with respect to E_{VAC}.[5] While the results of experimental studies on Si and GaAs support some of the above predictions,[6,7] experimental confirmation for the existence of such defects across different material systems and whether they are the underlying cause for the observed surface E_F pinning and bulk asymmetrical doping remain to be demonstrated. Among the extrinsic defects, the most extensively studied impurity is hydrogen because of its high diffusivity and reactivity with defects, dopants, and host atoms. While hydrogen can incorporate in lattices due to its prevalence in the precursor gases employed for growth, oxygen impurities, on the other hand, are ubiquitous in almost all types of lattices because of its incorporation from substrates used during epitaxy, background O_2 and H_2O vapor in the precursor gases, growth chamber, and device processing environments. Like hydrogen, oxygen is a versatile defect capable of forming strong bonds with both anionic and cationic lattice atoms. It is also an amphoteric defect that can act as a donor or an acceptor and is known to strongly complex with vacancies and other defects. Surprisingly, unlike the case of hydrogen, systematic studies to identify the underlying correlations and general trends in the measured oxygen impurity concentration, dopability, and reactivity among the various semiconductor classes have not been undertaken.

The present study attempts to fill this knowledge gap by undertaking a survey of the reported experimental values of the bulk oxygen defect energies and surface E_F position of oxygen-exposed surfaces with an aim to find universal trends and determine its underlying

cause. Analysis of the reported experimental values of defect energies and the E_F position in a broad range of group IV, III–V, II–VI, and I–III–VI_2 semiconductors reveals several commonalities between seemingly different semiconductor systems: (i) the surface E_F values of semiconductors exposed to ambient O_2 are universally constant at approximately −5.1 eV below E_{VAC}; (ii) substitutional oxygen defect levels in the bulk lattice of various semiconductors also exhibit a similar constant universal energy value of ∼−5.0 eV below E_{VAC}. It is shown that the universal surface E_F alignment is due to a process called surface transfer doping (STD),[8,9] wherein electrochemical reactions occurring in a nanoscale-adsorbed water film on the semiconductor surfaces cause the pining of the semiconductor E_F level at the energy of the oxygen reaction. The existence of this commonality between the electrochemical and physical energy scales and the presence of universal O-defect level has strong bearing on the doping characteristics of many semiconductors.

Figure 1 shows the band lineup of various sp^2- and sp^3-bonded semiconductors along with the reported experimental E_F values (work function) of semiconductors having physisorbed oxygen at the surface. The work function values along with the values of bandgap and electron affinities are summarized in Table I. Here, experimentally determined values of the work function, ϕ, were measured either by Kelvin probe under ambient air conditions or by ultraviolet photoelectron spectroscopy (UPS) from the secondary electron cutoff from samples previously exposed to oxygen or air. Alternatively, the absolute E_F position was determined through x-ray photoelectron spectroscopy (XPS) using the measured values of valence band (VB) offsets and band bending of oxygen-exposed surfaces and electron affinity values. All listed electron affinity values correspond to the value measured on clean surfaces under ultrahigh vacuum (UHV) conditions. Figure 1 shows the striking similarity of the measured E_F value of "oxygen-exposed" surfaces across different material systems, with most reported values falling within a narrow range between −4.8 and −5.2 eV. The observed scatter of several 100 meV in the E_F position may arises from several sources: (i) uncertainty in the electron affinity values, which is influenced by crystallographic orientation and surface polarity, of the tested sample; (ii) differences in the experimental test conditions (O_2 and H_2O concentrations) of various researchers; and (iii) differences in the work function of reference standards (e.g., ϕ of Au) used for calibration. Nevertheless, the observed narrow range of E_F values is remarkable considering the broad range of chemical and electronic properties of the semiconductors used here, which includes both covalent (groups IV and III–V alloys) and more ionic (II–VI alloys) in sp^2 and sp^3 bonding configurations, and whose bandgaps span an energy range of more than 6 eV. Therefore, one can conclude that ambient O_2 pins the E_F position of most semiconductors.

In addition to pinning the surface E_F to a constant universal value, analysis of the important point defects reported in several semiconductors shows that the substitutional oxygen-related defect present in the bulk of the lattice also exhibits a constant universal value of ∼−5 eV (Fig. 2). Oxygen and water vapor are also the two most ubiquitous residual impurities in any vacuum chamber, and whose concentration strongly dependent on the purity of precursor gases employed for film growth (e.g., H_2O contamination in NH_3), types of substrates

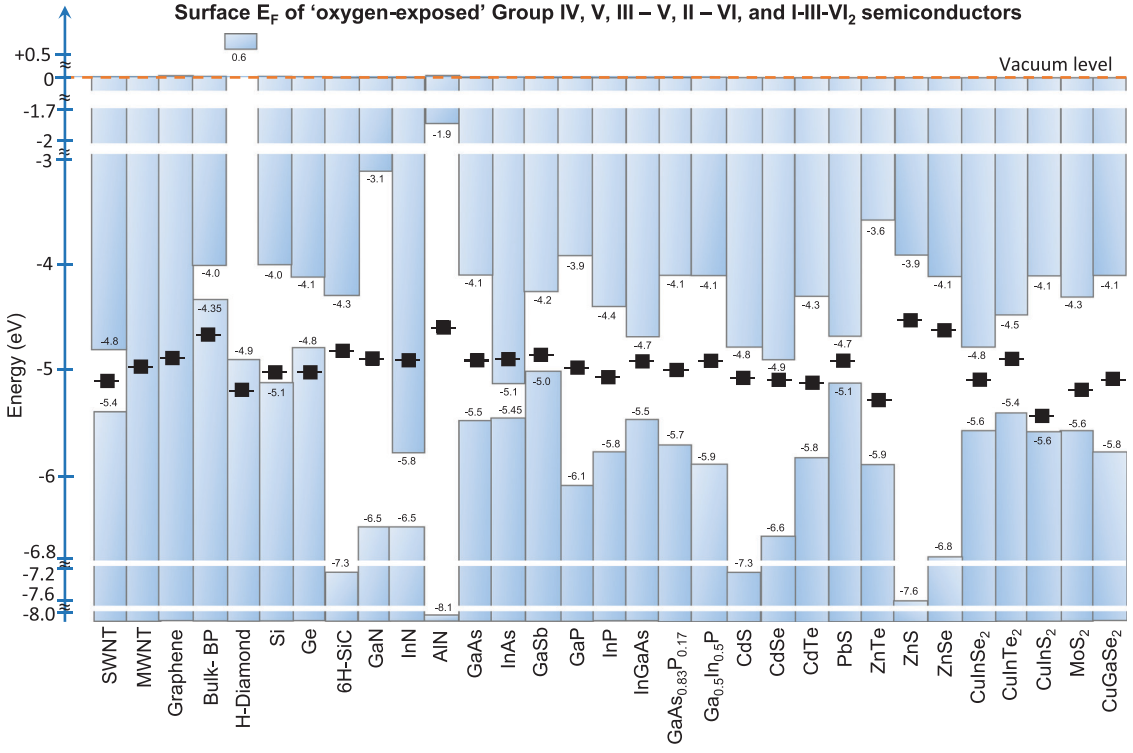

FIG. 1. Schematic diagram of the experimentally determined Fermi- and band edge energies of semiconductors showing the universality of the E_F value close to ∼−5.1 eV for "oxygen-exposed" surfaces. The reported values are summarized in Table I.

TABLE I. Reported experimental values of predominant oxygen defects in various IV, III–V, II–VI, and I–III–VI semiconductors along with the reported values of electron affinity (χ) and bandgap (E_g) of UHV-prepared semiconductor surfaces. All are experimental values unless explicitly noted. E_C = conduction band, E_V = valence band, ϕ = work function, and ML = monolayer.

Semiconductor (preferential doping)	E_g (eV)	χ (eV)	E_F of oxygen-exposed surface (eV)	O- and H-defect energies (eV)
Groups IV and V semiconductors				
Carbon nanotubes	Tunable	4.8[53] (in non-aqueous solution)	$\phi = 4.95$[54] (multi-walled) $\phi = 5.1$[54,55] (single walled)	Not established
Graphene	Metal	...	$\phi = 4.9$[56] (one and two layers)	Not established
Black phosphorus (BP, p)	0.35–1.7	4.0[57]	$\phi = 4.6$–4.75[19] (bulk and ML)	E_V −0.11 (Ref. 58) (ML, calculated)
Diamond	5.5	−1.3 τo −0.6[25] (H-terminated) 1.0–1.5[59] (O-terminated)	$\phi = 5.1$[9,25]	E_C −3.75[60] (inferred) OH:E_V +2.0[61] (calculated)
Si	1.12	4.0[62] (111)	$\phi = 5.0$[63]	E_V +0.32[64,65]
Ge	0.67	4.13[66,67]	$\phi = 5.0$[68] (100)	E_V +0.07[18]
6H-SiC	3.0	4.3[69]	$\phi = 4.8$[56]	E_C −0.87[70]
III–V semiconductors				
GaN (n)	3.4	3.1–3.4[31,32]	E_C −1.8[38] E_C −1.4[39]	O_N:E_C −0.033 (shallow donor) O_N–V_{Ga}: E_C −2.1 eV (Ref. 71) H: E_V +2.4 (theoretical, Ref. 5)
InN (n)	0.7	5.8–6.0[40,41] (using χ_{AlN} + ΔE_C offset)	∼E_C +0.9[72,73]	E_C +0.9 (O ∼5 × 10^{20})[17]
AlN (insulating)	6.2	1.9[74,75]	E_V +3.5 eV[69]	O_N–V_{Al}: E_C −3.1(−3.3)[12,76,77]
GaAs (n)	1.42	4.1[33]	E_C −0.65 (−0.8)[78,79]	E_C −0.825[50] E_C −0.74[80] O_{As}: E_C −0.79[81] H: E_C −0.13[7]
InAs (n)	0.35	5.1[33]	E_C +0.2[82]	O_{As}: E_C +0.17[45]
$In_{0.5}Ga_{0.5}As$	0.76	4.7[82]	E_C −0.2[82]	Not established
GaP	2.24	3.8[33] 3.96[83]	$\phi = 4.95$[84] E_C −1.2[84]	O_P: E_C −0.9[85,86] (deep donor) T5: E_C −0.97[87]
GaSb	0.7	4.2[33]	E_C −0.65[78]	Not established
InP	1.42	4.43[88] 4.3–4.4[89,90]	E_C −0.52(−0.72)[91]	O: E_C −0.47[92] H: E_C +0.05[7]
$Al_{0.5}In_{0.5}P$	2.36[93]	3.78[94]	Not available	O: E_C −0.65;[95] O <10^{17} cm^{-3} E_C −0.89; O >10^{17} cm^{-3}
GaAsP	1.61–1.64[96]	4.1[97]	$\phi = 5.02$[84]	$GaAs_{0.9}P_{0.1}$ O: E_C −0.8[96] $GaAs_{0.83}P_{0.17}$ O: E_C −0.82 and E_C −1.2[96]
$Ga_{0.5}In_{0.5}P$	1.85[90,98]	4.09[90,94]	E_C −1.15 or $\phi = 4.9$[99]	E_C −0.63 (−0.82 eV)[100]
$Al_{0.1}Ga_{0.9}As$	1.55[101]	3.96[101]	Not available	O: E_C −0.56; E_C −0.8[102–104]
$(Al_{0.3}Ga_{0.7})_{0.51}In_{0.49}P$	2.1[98]	3.9[98,105]	Not available	O: E_C −1.0[106]
II–VI and I–III–VI_2 and other semiconductors				
CdS (n)	2.47	4.79[107] 4.8[108]	E_C −0.3[109]	O_S: E_C −0.5[110]
CdSe (n)	1.7	4.9–4.98[107,108]	E_C −0.14[111]	Not established

TABLE I. (*Continued.*)

Semiconductor (preferential doping)	E_g (eV)	χ (eV)	E_F of oxygen-exposed surface (eV)	O- and H-defect energies (eV)
CdTe (n)	1.5	4.28[107]	E_C −0.85 or $\phi = 5.1$[112]	O_{Te}–H: E_C −0.73 (theoretical[113]) $E_{Trap} = 0.78$[114] H: E_C −0.07[7]
PbS	0.41	4.6–4.7[115–117]	$\phi = 4.9$[118]	O: E_C −0.23[119,120]
ZnTe (p)	2.26	3.6[107,121,122]	E_C −1.7[123]	Not established E_C −0.73[124] E_C −0.5[125] (high O-doping forms intermediate band)
ZnS (n)	3.7	3.9[107]	$\phi = 4.5$[126]	O_S related: E_C −0.92[127]
ZnSe (n)	2.67	4.09[107]	E_C −0.5[123]	O_{Se} related: E_C −0.83[128]
$CuInSe_2$ (p/n)	1.02	4.6[129]	$\phi = 5.0$–5.1[130,131]	E_C −0.28 (inferred[132]) E_C −0.2 (theoretical[133])
$CuGaSe_2$ (p)	1.68	4.1[134]	$\phi = 5.1$[135]	Not established
$CuInTe_2$ (p)	0.92	4.5[136]	$\phi = 4.85$[137]	Not established
$CuAlSe_2$ (p)	2.68	3.8[138]		E_C −0.6[139]
$CuInS_2$ (p)	1.5	4.1[131,140]	$\phi = 5.5$[141]	E_C −0.7 (theoretical[142]) annihilates e^- donors[143] H:E_V +1.41 (theoretical[144])
MoS_2	1.3	4.3[145]	$\phi = 5.2$–5.4[146]	Not established

(sapphire and quartz) as well as the base pressure of the growth chamber.[10] At the higher substrate temperature employed during the growth process, the background H_2O and O_2 can absorb at local defects, such as vacancies and dangling bonds at the grain boundaries, where they can undergo dissociation, and eventually incorporate into the bulk lattice. Experimental determination of elemental defect concentration shows that oxygen is one of the most prevalent impurities in semiconductors. For example, oxygen concentration of up to $\sim 10^{19}\,cm^{-3}$ has been reported in GaN films grown by ammonothermal, and high pressure processes without any additional oxygen in the precursor gases.[11] AlN represents an extreme case in III–V alloys as oxygen concentrations in excess of 4 at. % have been noted,[12] which is consistent with theoretical calculations[13] that show O can easily substitute for N. Similarly, the significance of "persistent universal oxygen" incorporation in II–VI semiconductor lattices was noted by Bube in early 1950s,[14] and the study reported the profound influence of oxygen on the photoelectronic properties of CdS and CdSe. More recently, Barja and co-workers[15] reported the prolific presence of substitutional oxygen defects in monolayer (ML) transitional metal dichalcogenides of $MoSe_2$ and WS_2.

Table I and Fig. 2 summarize the reported experimental energy levels of substitutional O-related defects in various groups IV and III–V [Fig. 2(a)], and II–VI and I–III–VI_2 [Fig. 2(b)] semiconductors with respect to the conduction band (CB) or VB positions. In cases where the O-defect level position at different oxygen concentrations was reported, the energy level corresponding to the highest concentration was used for analysis. Using the listed electron affinity values of clean UHV surfaces for all semiconductors, the absolute energy position of the reported O-defect energies was determined and used for generating Fig. 2.

Several key features are evident from Fig. 2. The energy level of the substitutional bulk O-defect also lies within the narrow energy range of −4.9 to −5.2 eV below E_{VAC}. Interestingly, this average O-defect level of ∼−5.0 eV in the bulk is very close to the energy of the surface E_F position (−5.1 eV) pinned due to physisorbed oxygen shown in Fig. 1. Again, bandgaps considered for the analysis have a broad energy span of 0.35–6.2 eV. In wide bandgap semiconductors like GaAs, AlN, and most other III–V alloys, the O-defect lies at the midgap energies and acts as a deep-level acceptor that causes e^- depletion in the native n-type lattice. In fact, the deep character of O-defect in AlN explains the fact that even a large oxygen concentration does not lead to n-type conductivity, the material remains an insulator with a high activation energy of 2.1 eV necessary for electrical conductivity.[16] In materials such as InN and InAs, the position of O-defect lies well within the CB, where it serves as a donor causing e^- injection at the CB edge.[17] In contrast, O-defect energy lies either close to or well within the VB in germanium and black phosphorus (BP), where it enhances the p-type doping of the lattice.[18,19] Thus, O is a versatile defect that can be both a donor and an acceptor (amphoteric) defect in semiconductors.

The underlying cause for the universality of the O-level is not clear. A similar universality has been previously noted with transition metal ion impurities in certain classes of semiconductors,[20] where the highly localized *d*-shell energy levels of transition metals become insensitive to the host lattice. In fact, this constancy of the *d*-shell energy level has been exploited for deducing the band edge offsets by aligning the known levels of transition metal impurities in different semiconductors.[21] This localized defect theory may not be valid in the present case as both oxygen and hydrogen can strongly bond with lattice atoms. Instead, an alternative

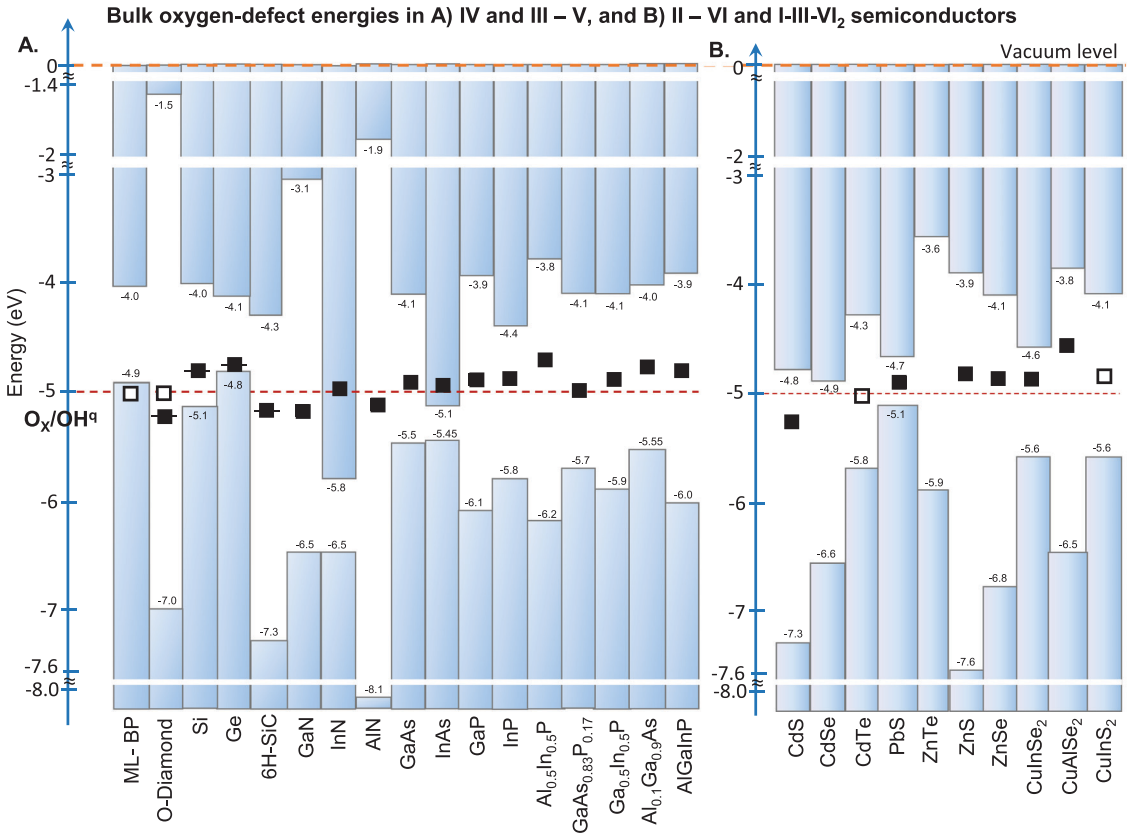

FIG. 2. Reported experimental (solid symbol, ■) and theoretical (open symbol, □) values of the predominant bulk oxygen-defect energies in IV and III–V (a), and II–VI and I–III–VI_2 (b) semiconductors along with the CB and VB positions of UHV-prepared surfaces. See Table I.

explanation based on the previously observed phenomenon of surface transfer doping is proposed.

First, the universal surface E_F pinning by physisorbed ambient O_2 doping is considered. A situation where the E_F in the semiconductor is naturally and spontaneously pinned by charge injection occurs when clean UHV-grown surfaces are exposed to humid ambient air, where O_2 and adsorbed water act as dopants for the semiconductor surface through the process of surface transfer doping (STD). This phenomenon was first discovered the hydrogenated diamond,[8,22] where it was shown to induce a p-type surface conductivity under ambient air conditions in otherwise insulating bulk lattice. A thin water film, which naturally condenses on most surfaces exposed to humid conditions,[23] containing ambient dissolved gases and ions enables an electrochemical reaction that acts as an external donor/acceptor for the electrons in the underlying semiconductor. Under ambient atmosphere, oxygen is one of the major constituents that has the right energetics for electron exchange through the electrochemical reaction:[9,24]

$$O_{2,\mathrm{film}} + 4H_3O^+_{\mathrm{film}} + 4e^- \leftrightarrow 4H_2O_{\mathrm{film}} \quad (E_{O_2/H_2O} = -5.2\,\mathrm{eV}). \quad (1)$$

Under atmospheric conditions, the electrochemical potential of electrons of reaction (1), $\bar{\mu}_{efilm} = E_{O_2/H_2O}$, is equal to −5.2 eV below E_{VAC}. For $E_F > \bar{\mu}_{efilm}$, the redox reaction acts as an acceptor [forward reaction (1)] for e^- in the semiconductor, and conversely as a donor [reverse of reaction (1)] when $E_F < \bar{\mu}_{efilm}$. In the case of hydrogenated diamond, its low χ of −0.6 eV (Ref. 25) puts the E_F above $\bar{\mu}_{efilm}$ (Fig. 3). Consequently, STD by ambient oxygen gives rise to a hole accumulation layer and a p-type conductivity. On most semiconductors, the adsorbed water is present only on the surface, which restricts the space charge region to the surface/near-surface region. This, however, is not the case with many transition metal oxides, which have large voids in their structure that accommodate interstitial lattice H_2O and H^+, and therefore can enable bulk doping through STD.[26]

Since its first discovery in diamond, STD has been observed in several different semiconductors and is summarized in Fig. 3. STD by ambient O_2 and H_2O has been shown to be responsible for the p-type surface conductivity in semiconducting single-walled nanotubes (SWNT),[9,27–29] graphene,[30] and activated carbon fibers for which $E_F > \bar{\mu}_{efilm}$. In lower electron affinity semiconductors such as GaN [$\chi = 3.1$–3.4 eV (Refs. 31 and 32)] and GaAs [$\chi = 4.1$ eV (Ref. 33)], the $\bar{\mu}_{O_2/H_2O}$ lies near the reported[34] midgap energies, and therefore, the ambient oxygen can act as acceptors for the CB electrons of the native n-doped lattice and leads to the formation of an electron depletion region at the surface.[35,36] Indeed, experimental evidence shows that the E_F of a clean stoichiometric GaN lattice shifts from E_C −0.3 eV (Refs. 31 and 37) to a value of ∼E_C −1.8 eV (Refs. 38 and 39) upon exposure to ambient air. The small value of 0.2–0.3 eV residual band bending seen on clean adsorbate-free surfaces is due to native

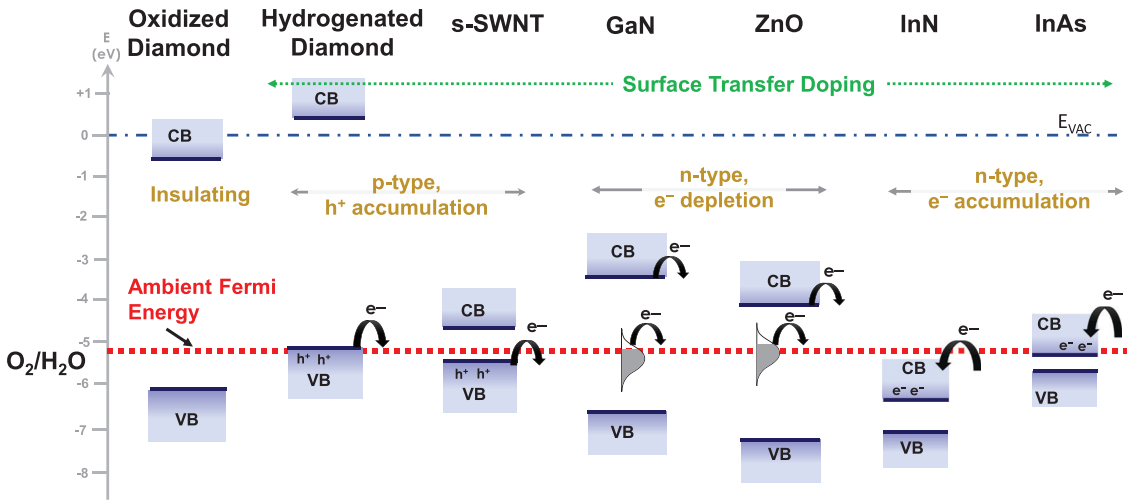

FIG. 3. Schematic diagram showing the Fermi- and band edge energies of semiconductors that show spontaneous surface transfer doping phenomenon under ambient air. The $\overline{\mu}_{efilm} = E_{O_2/H_2O}$ is −5.2 eV below E_{VAC} (denoted as ambient Fermi energy) for oxygen partial pressure of 0.21 bar and pH of the water film of 7. All values are before electronic contact. The curved arrow indicates the direction of electron exchange between the semiconductor and the adsorbed water film that gives rise to various types of space charge layer in addition to the any intrinsic space charge layer formed due to surface states. The approximate energy range of the midgap states reported in GaN and ZnO[34,35] is also shown.

acceptor defects. Therefore, the STD by ambient O_2 causes E_F of GaN (work function, $\phi = 5.0$ eV) to be fixed near the energy position of E_{O_2/H_2O}. In contrast to GaN and GaAs, both InN and InAs have unusually high electron affinities (χ): $\chi_{InN} = 5.8$ eV[40,41] and $\chi_{InAs} = 5.1$ eV,[33] and both have an electron accumulation layer on the surface. Recent results[42] show that moderate UHV annealing up to 340 °C, which enables desorption of physisorbed ambient species, can dramatically reduce the band bending seen in "air-exposed" samples. Therefore, the formation of electron accumulation in InN and E_F pinning at −4.9 eV was attributed primarily to STD by ambient oxygen acting as donors.

Similar effects of ambient O_2 have been noted in a wide range of semiconductors, including many transition metal dichalcogenides and oxides,[26,43] ZnS,[44] CdS, CdSe,[14] InAs,[45] GaAs,[46] and MoS_2.[47] Therefore, the E_F pinning in semiconductors exposed to ambient air is likely due to the universal charge transfer process with the quasi-infinite source of ambient O_2 that fixes the E_F of the semiconductor near its redox energy value of −5.2 eV under ambient conditions.

Next, the possible cause for the universal bulk O-defect level is considered. At the higher substrate temperature employed during the growth, a uniform adsorbed water film is unlikely. However, the background H_2O vapor and O_2 can absorb at local vacancy sites and eventually incorporate into the bulk lattice. Given that the substitutional bulk O-defect level (−5.0 eV) is close to the value of surface E_F position (−5.1 eV) pinned by physisorbed O_2 redox reaction, it is hypothesized that the mechanism giving rise to an energetically common O-defect level in semiconductors may be related to the STD process occurring in the bulk during the growth. It is likely that dissociated species of oxygen and water vapor present during the growth may incorporate into the bulk vacancy sites according to the defect reaction,

$$O_X^q + H_i + e^- \leftrightarrow (O_X H_i)^{q-1}, \tag{2a}$$

$$O_X^q + H_i \leftrightarrow (O_X H_i)^{q+1} + e^-. \tag{2b}$$

Here, O_X^q represents the oxygen defect with charge state q substituting for the lattice (X) atom site and H_i is a mobile interstitial hydrogen defect in the vicinity of O_X^q. The existence of this type of defect complexes including $(O_X Li_i)^{q\pm1}$ and $(Si_X H_i)^{q\pm1}$ has been demonstrated in germanium.[48,49] Here, the $O_X^q/(O_X H_i)^{q\pm1}$ is an amphoteric defect complex that can serve as both a donor and an acceptor. For instance, both experimental[50] and theoretical[13] results show that in GaAs, AlN, and many other III–V alloys, the O-defect lies at the midgap energies and acts as a deep level acceptor that causes e^- depletion in the native n-type lattice. Calculations show that O can easily substitute for As in GaAs and N in AlN and has a midgap energy level that causes depletion of electrons from the native lattice. The acceptor-type behavior of the O-defect can arise from reaction (2a). In contrast, the donor-type behavior of O-defect in InN is due its position well within the CB, which causes degenerative n-doping of the lattice. This can be rationalized using reaction (2b), where the same defect complex, $O_X^q/(O_X H_i)^{q\pm1}$, acts as electron donors. In AlN, the deep position of O-defect makes n-type conductivity difficult. Thus, it is neither a donor nor an acceptor, and the material remains an insulator.[16] Therefore, the universality of the O-defect in the semiconductor maybe due to the amphoteric $O_X^q/(O_X H_i)^{q\pm1}$ complex. Similar to surface physisorbed O_2, the presence of high concentration of substitutional bulk O-defect can gate charge carriers from the intentionally introduced dopants, and this may be the reason for the observed asymmetrical doping in many wide bandgap semiconductors. Finally, it has been noted that in heavily ion-bombarded samples, the E_F of the material stabilizes at a universal value of −4.9 eV.[51] This value is close to the value of bulk and surface oxygen levels reported here. While amphoteric native defects have been speculated as the cause for E_{FS}, it is more likely that facile oxygen uptake occurring in the ion-damaged samples even when stored under UHV conditions[52] pins the E_F close to −5 eV.

In conclusion, it is shown that ambient O_2 and water vapor have a profound impact on both the surface and bulk electronic properties through the process of STD. Surface doping leads to the pinning of the surface Fermi level universally at approximately −5.1 eV across several material systems. Similarly, analysis of the substitutional bulk oxygen defect in a wide range of semiconductors shows that they have a universal energy of ∼−5.0 eV below E_{VAC}. This universal alignment of the O-defect level can serve as a reference scale for the band edge alignment similar to transition metal in semiconductors.

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DATA AVAILABILITY

The data that support the findings of this study are available within the article.

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